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## Equilibrium and kinetic models for colloid release under transient solution chemistry conditions

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## ABSTRACT

We present continuum models to describe colloid release in the subsurface during transient physicochemical conditions. Our modeling approach relates the amount of colloid release to changes in the fraction of the solid surface area that contributes to retention. Equilibrium, kinetic, equilibrium and kinetic, and two-site kinetic models were developed to describe various rates of colloid release. These models were subsequently applied to experimental colloid release datasets to investigate the influence of variations in ionic strength (IS), pH, cation exchange, colloid size, and water velocity on release. Various combinations of equilibrium and/or kinetic release models were needed to describe the experimental data depending on the transient conditions and colloid type. Release of *Escherichia coli* D21g was promoted by a decrease in solution IS and an increase in pH, similar to expected trends for a reduction in the secondary minimum and nanoscale chemical heterogeneity. The retention and release of 20 nm carboxyl modified latex nanoparticles (NPs) were demonstrated to be more sensitive to the presence of  $\text{Ca}^{2+}$  than D21g. Specifically, retention of NPs was greater than D21g in the presence of 2 mM  $\text{CaCl}_2$  solution, and release of NPs only occurred after exchange of  $\text{Ca}^{2+}$  by  $\text{Na}^+$  and then a reduction in the solution IS. These findings highlight the limitations of conventional interaction energy calculations to describe colloid retention and release, and point to the need to consider other interactions (e.g., Born, steric, and/or hydration forces) and/or nanoscale heterogeneity. Temporal changes in the water velocity did not have a large influence on the release of D21g for the examined conditions. This insensitivity was likely due to factors that reduce the applied hydrodynamic torque and/or increase the resisting adhesive torque; e.g., macroscopic roughness and grain–grain contacts. Our analysis and models improve our understanding and ability to describe the amounts and rates of colloid release and indicate that episodic colloid transport is expected under transient physicochemical conditions.

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### 1. Introduction

An understanding of and an ability to accurately predict the release of colloids (including microorganisms, particulate organic matter, clay, metal oxides, and nanoparticles) in porous media are needed for many agricultural, environmental, and

industrial applications. Under steady-state flow and solution chemistry conditions low amounts of colloids are slowly released from the solid phase when the kinetic energy of diffusing colloids exceeds the adhesive interaction energy (Ryan and Elimelech, 1996; Ryan and Gschwend, 1994; Shen et al., 2007). Conversely, significant amounts of colloid release may rapidly occur during temporal changes (i.e., transients) in solution chemistry (Grolimund et al., 2001; Roy and Dzombak, 1996) and/or water velocity (Bergendahl and Grasso, 1998,

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2000). These observations indicate that different mechanisms control colloid release during steady-state and transient conditions. Transient physicochemical conditions may occur in the subsurface as a result of infiltration and recharge, groundwater and surface water interactions, injection and/or extraction wells, and contamination events.

Colloid immobilization and release at a particular location on the collector surface depend on the strength of the resisting adhesive torque in comparison to the applied hydrodynamic torque (Bergendahl and Grasso, 1998, 2000), and the adhesive interaction energy relative to the kinetic energy of diffusing colloids (Shen et al., 2007; Simoni et al., 1998). Transients in water velocity alter the hydrodynamic force that acts on immobilized colloids (Bergendahl and Grasso, 1998, 2000), and is spatially variable because of the complex geometry of the pore space (Bradford et al., 2011). Transient solution chemistry conditions impact the adhesive force by altering the macroscopic zeta potentials and the electric double layer thickness (Grolimund and Borkovec, 2006; Ryan and Elimelech, 1996). In addition, the dependence of the adhesive force on solution ionic strength (IS) is a function of the colloid size and the nanoscale heterogeneity (e.g., the distribution of charge and roughness) within the zone of electrostatic influence (Bendersky and Davis, 2011; Duffadar and Davis, 2007). Natural colloid and solid surfaces always exhibit some degree of nanoscale heterogeneity due to surface roughness, mineral defects, isomorphic substitution, protonation/deprotonation of hydroxyl groups, and adsorption of different ions, organics, and clay particles (Suresh and Walz, 1996; Tufenkji and Elimelech, 2005; Vaidyanathan and Tien, 1991). Consequently, spatial variability of the adhesive force is also expected. The above information indicates that transient physicochemical conditions initiate colloid release by altering the force and/or torque balance that acts on immobilized colloids, and that only a fraction of the retained colloids may be released because of spatial variations in the adhesive and hydrodynamic forces and torques.

Several continuum models have been developed to simulate colloid release during transients in solution chemistry (Bedrikovetsky et al., 2011; Bradford et al., 2012; Grolimund and Borkovec, 2006; Lenhart and Sayers, 2003; Tosco et al., 2009). In general, colloid transport equations are coupled to the solution chemistry through explicit dependencies of retention and/or release parameters on solute concentrations (e.g., IS, pH and/or adsorbed divalent cations). The transport equations for solution chemistry and colloids are subsequently solved and colloid transport parameters are updated at each time step. All of the continuum models employ different first-order kinetic formulations for colloid retention and release; e.g., some considered population heterogeneity, blocking, or multiple retention sites. In addition, the functional dependency of retention and release parameters on solution chemistry varies significantly among the models. Only some of these models can be easily extended to describe colloid release with transients in water velocity (Bedrikovetsky et al., 2011; Bradford et al., 2012).

One challenge in continuum modeling of colloid release is determining the amount of colloid release with the physicochemical perturbation. A finite number of colloids can be retained in porous media under steady-state conditions. The maximum solid phase concentration of retained colloids ( $S_{max}$ ) is obtained when all retention sites are filled. Under steady-state

conditions, the value of  $S_{max}$  can be determined by direct microscopic observations in simplified systems (Adamczyk et al., 1992), inverse optimization of experimental breakthrough curve data that exhibit blocking behavior (Adamczyk et al., 1994; Johnson and Elimelech, 1995), or theoretically estimated from torque balance calculations (Bradford et al., 2013). Experimental and theoretical results demonstrate that  $S_{max}$  is sensitive to the solution chemistry and hydrodynamic conditions (Adamczyk et al., 1995; Bradford et al., 2013; Sasidharan et al., 2014). Such changes in  $S_{max}$  with physicochemical conditions have been related to the amount of colloid release during transient conditions (Bedrikovetsky et al., 2011; Bradford et al., 2012). However, the dependence of  $S_{max}$  on physicochemical conditions is more complicated during colloid release than retention because some of the retained colloids cannot be released by a given perturbation (e.g., irreversible retention) (Adamczyk et al., 1992). The functional dependence of  $S_{max}$  on IS therefore exhibits hysteresis during retention and release phases (Bradford et al., 2012). The importance of temporal changes in  $S_{max}$  with transient conditions on colloid release is not widely appreciated, and has not yet been incorporated into continuum models that account for the full range of equilibrium and/or kinetic release behavior.

A second challenge in continuum modeling of colloid release with transient physicochemical conditions is describing the dynamics of colloid release. The adhesive interaction at a particular location on the collector surface may change with a physicochemical perturbation as ions transfer and/or react in the gap separating the colloid from the collector surface. Spatial variations in the adhesive (and associated separation distances) and hydrodynamic forces produce a distribution of mass transfer and reaction rates for ions on collector surfaces. Indeed, various combinations of equilibrium or kinetic models are needed to describe geochemical reactions of specific ions in soils (Mayer et al., 2002; Šimůnek and Valocchi, 2002). Similarly, colloid release with transients has sometimes been observed to occur slowly and at other times very rapidly (Bedrikovetsky et al., 2011; Bradford et al., 2012; Grolimund and Borkovec, 2006; Khilar and Fogler, 1984; Lenhart and Sayers, 2003; Shen et al., 2012; Torkzaban et al., 2013; Tosco et al., 2009). It is therefore logical to anticipate that equilibrium, kinetic, combined equilibrium and kinetic, or even two-site kinetic models may be needed to describe colloid release under transient physicochemical conditions. However, continuum models for colloid release have not yet been developed to describe all of these possible conditions.

The overall objective of this research is to improve our understanding of and ability to simulate colloid release under transient physicochemical conditions. This aim is accomplished by relating the amount of colloid release with transients to changes in  $S_{max}$ , and then developing equilibrium, kinetic, combined equilibrium and kinetic, and two-site kinetic models to describe a wide variety of observed colloid release behavior. These continuum models were subsequently applied to experimental colloid release datasets under various transient conditions to investigate the influence of IS, pH, cation exchange, colloid size, and water velocity on release. Analysis of these data improves our knowledge of fundamental factors influencing colloid release during transient physicochemical conditions, and helps to identify the proper model formulations to describe such behavior.

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